

**Table S1:** Contacts of the residues of the VgrG1-ACD N-terminus with the core of the enzyme in the apo- and holo- forms. The distances are given in Å. Hb : hydrogen bond; sb : salt bridge ; vdw : van der Waals interaction. ASA : accessible surface area ; BSA : buried surface area. Nv : not visible.

N-term	Core apo	Distance / type	BSA/ASA (%)	Core holo	Distance / type	BSA/ASA (%)
Thr -2	Lys 260	2.74 / hb	60	nv	nv	-
Lys -1	Glu 18	2.50 / sb	85	nv	nv	-
Ala 0	Gln 32	3.3 /vdw	45	Thr 133	3.5 / vdw	21
Thr 1	Arg 268	3.20 / hb	83	Lys 33	3.5 / vdw	82
Pro 2	Val 80	3.7 / vdw	82	Tyr 82	2.67/ hb	57
Asp 3	Asn 323	2.72 / hb	40	-	-	8
Phe 4	Tyr 82	3.3 / vdw	42	ATP	3.6 / vdw	58
Pro 5	Asn 323	3.2 / vdw	33	-	-	52
Total buried surface :			570 Å <sup>2</sup>	324 Å <sup>2</sup>		